

FIG. 1

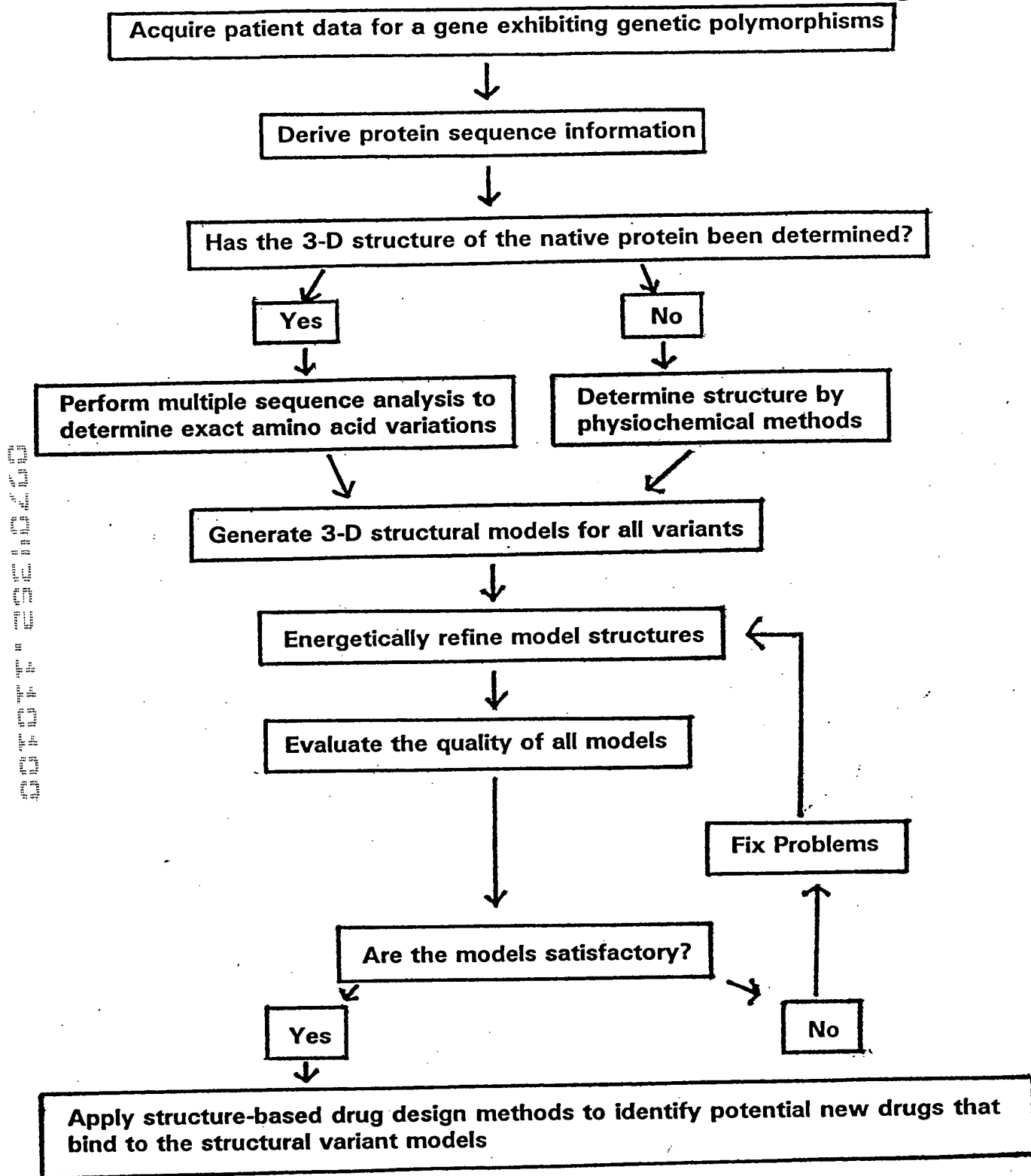


FIG. 2

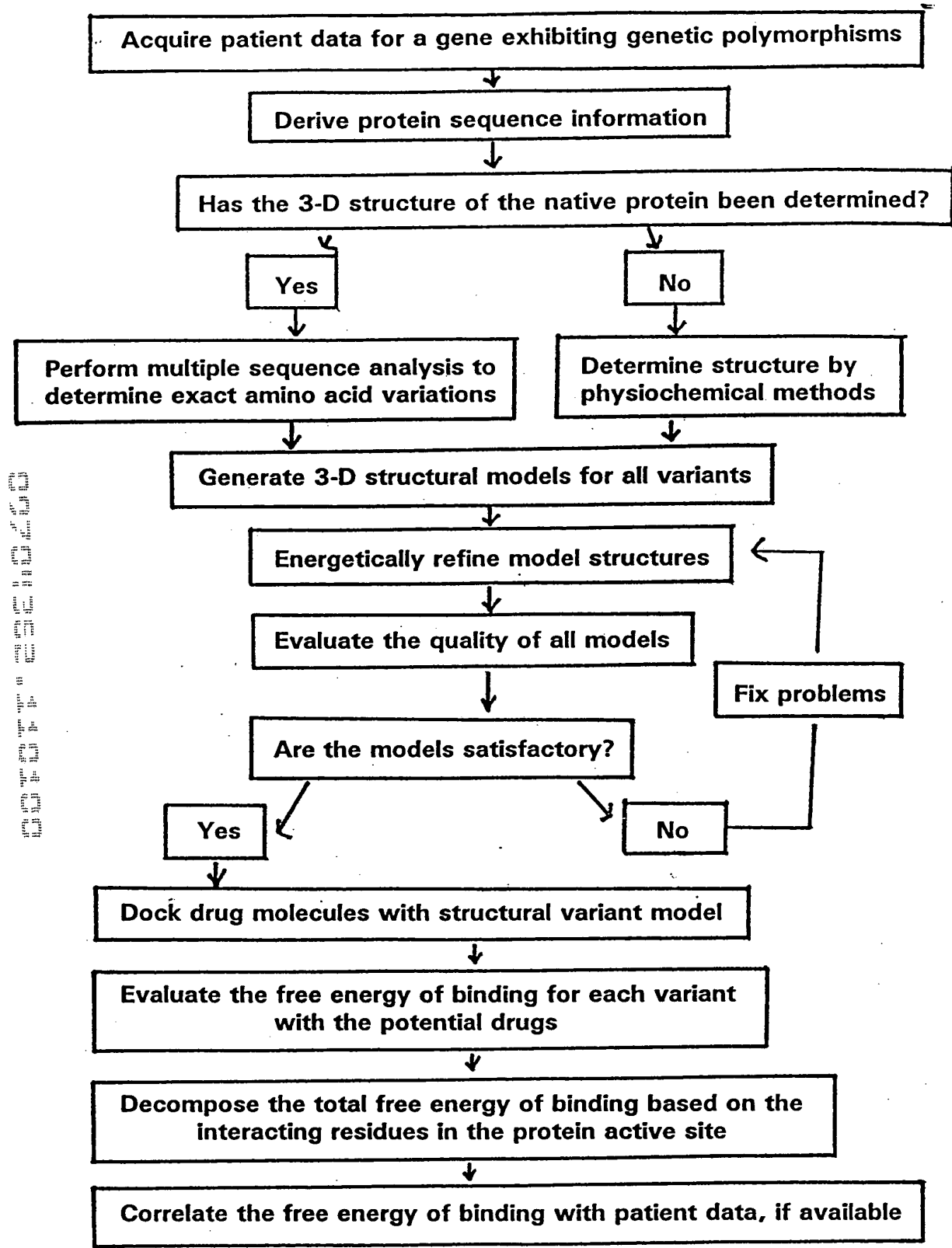
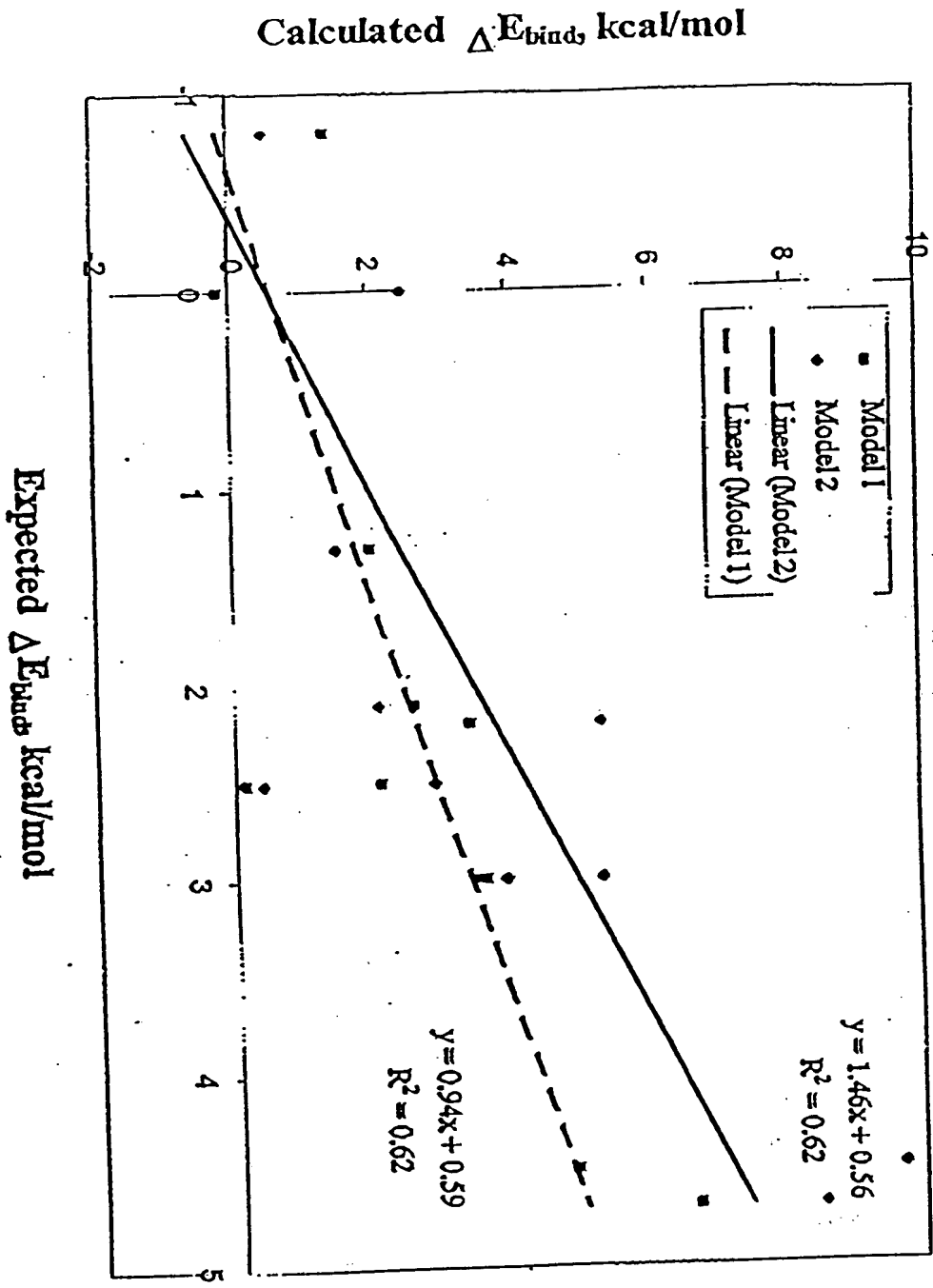


FIG. 3

FIG. 4

Correlation between Experimental and Calculated Changes  
of Binding Energy upon Ligand Modifications in the Binding  
Site of NS3



# Comparison of Calculated versus Experimental Binding Free Energy Changes

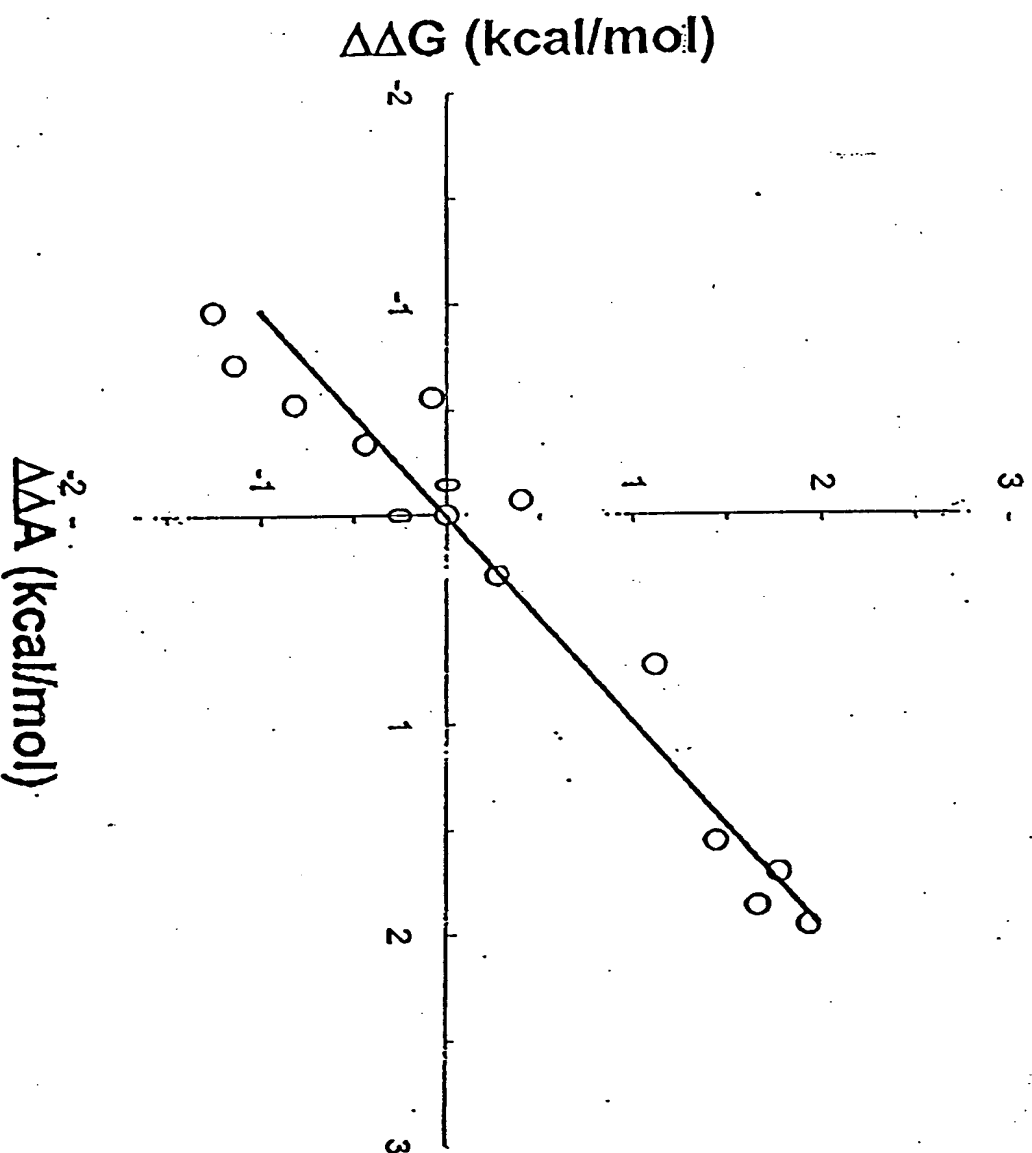


FIG. 5